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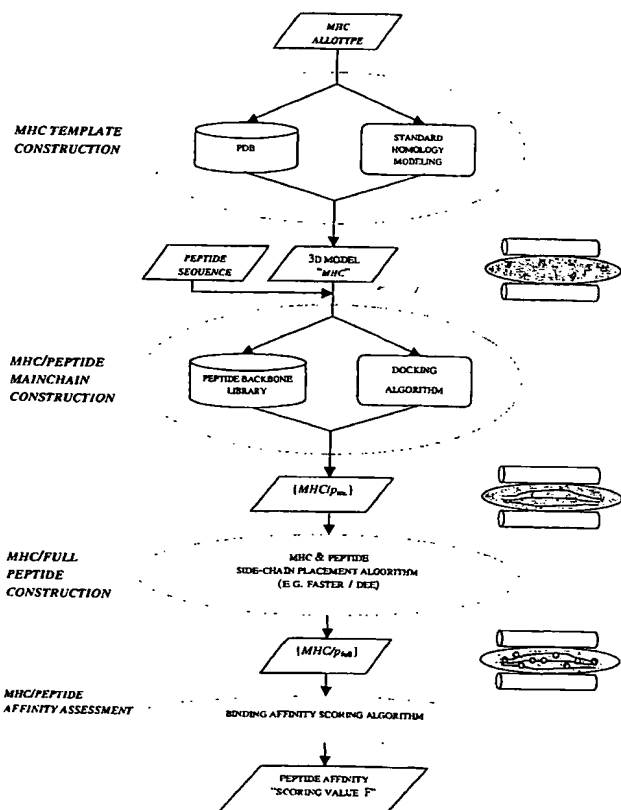
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[Continued on next page]

(54) Title: METHOD FOR PREDICTING THE BINDING AFFINITY OF MHC/PEPTIDE COMPLEXES



(57) Abstract: The present invention relates to a method for structure-based prediction of properties of peptides and peptide analogs in complex with major histocompatibility (MHC) class I and class II molecules. The said properties mainly relate to the three-dimensional structure of an MHC/peptide complex and the binding affinity of a peptide for an MHC receptor. The invention further relates to a computer program and a device therefor. The invention further relates to data produced by a method of the invention. The invention further relates to peptides and peptide analogs predicted to bind to target-MHC molecules. The present invention thus relates to the field of immunology, with possible applications in manufacture of vaccines, de-immunization of proteins, and manufacture of therapeutic agents, especially immunotherapeutic agents.

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SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

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INTERNATIONAL SEARCH REPORT

International Application No.

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A. CLASSIFICATION OF SUBJECT MATTER

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According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, BIOSIS, WPI Data, INSPEC

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	WO 98/59244 A (BROOKS TONY ;ECLAGEN LTD (GB); KEMP GRAHAM (GB); CARR FRANK (GB);) 30 December 1998 (1998-12-30) cited in the application page 4, line 27 - page 5, line 2 page 8, line 36 - page 9, line 9 claims 30,31 ----- -/--	1-46

☒ Further documents are listed in the continuation of box C.☒ Patent family members are listed in annex.

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"A" document defining the general state of the art which is not considered to be of particular relevance

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"&" document member of the same patent family

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	<p>KNEGTEL RONALD M A ET AL: "Molecular docking to ensembles of protein structures." JOURNAL OF MOLECULAR BIOLOGY, vol. 266, no. 2, 1997, pages 424-440, XP002944096 ISSN: 0022-2836 page 424, right-hand column, line 21 - page 425, left-hand column, line 14 page 425, left-hand column, line 32 - line 50</p>	1-46
Y	<p>MARELIUS JOHN ET AL: "Sensitivity of an empirical affinity scoring function to changes in receptor-ligand complex conformations." EUROPEAN JOURNAL OF PHARMACEUTICAL SCIENCES, vol. 14, no. 1, August 2001 (2001-08), pages 87-95, XP002227633 ISSN: 0928-0987 page 88, left-hand column, line 3 - line 14 page 93, left-hand column, line 8 - line 16</p>	1-46
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A	<p>DESJARLAIS JOHN R ET AL: "Computer search algorithms in protein modification and design." CURRENT OPINION IN STRUCTURAL BIOLOGY, vol. 8, no. 4, August 1998 (1998-08), pages 471-475, XP002227635 ISSN: 0959-440X page 472, right-hand column, line 29 - line 39</p>	1-46
A	<p>US 6 226 603 B1 (LUQUE IRENE ET AL) 1 May 2001 (2001-05-01) column 2, line 41 - line 57 column 9, line 22 - line 55</p>	1-46

INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

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